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United States Environmental Protection Agency
Washington, DC 20460

E. White

ORIGINAL

Document Description

SAT L-07-290

Date

7/20/07

STRUCTURE ACTIVITY TEAM REPORT

ver. 04/98

Case #:	L-07-0290	DCN:
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SAT Date:	6/29/2007	SAT Chair:
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Submitter: Tracerco

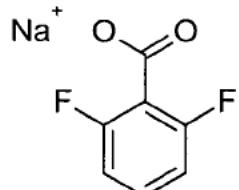
Chemical Name:

Benzoic acid, 2,6-difluoro-, sodium salt (1:1)

CAS RN:	6185-28-0	Trade Name:
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Tracerco 158c

Structure



6 0 0 7 0 0 0 2 1 6 2

Molecular Formula: C₇H₃F₂NaO₂

Molecular Wt. 180 WT%<500: WT%<1000:

MP: BP: >500 Eq. Wt:

H₂O Sol (g/L): >200 V.P. <0.000001

Max. Prod. Volume (kg/yr): 1000 Physical State: Solid

USE:

Tracer chemical to measure flow in deep oil-bearing strata. Concurrently submitted similar cases L-07-290 and L-07-292 to L-07-295. Analog L-07-271 has this same use. There is one reference in file CA on STN, a toxicity study.

P2REC. CRSS forward P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold Band Status by European regulatory authorities.

Related Case Numbers	Case Role	Related Case Numbers	Case Role
L-07-271		[REDACTED]	
[REDACTED]		[REDACTED]	
[REDACTED]		[REDACTED]	

Focus Date: JUL 9 2007

Results:

Conditional Grant P2REC ->

STRUCTURE ACTIVITY TEAM REPORT 29 June 2007

CASE NUMBERS: L07-0290 to L07-~~0290~~³⁰⁰

L07-0290 (F2)
L07-0291 (F)
L07-0292 (F2)
L07-0293 (F2)
L07-0294 (F2)
L07-0295 (F2)
L07-0296 (F4)
L07-0297 (F3)
L07-0298 (CF3)
L07-0299 (CF3)
L07-0300 (CF3)

P2REC: substitute for radionuclide tracers

RELATED CASES:

L07-0271 (F)



CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 1-2 1

KEYWORDS: DEVEL, LIVER, KIDNEY, SENS-ASTHMA, MUTA

SUMMARY OF ASSESSMENT:

FATE: MW162 to 216
solids with mp for L070271 (F) = 126 °C (M)
log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI),
1.59 to 3.10 (M)
log Kow for L070271 = -5.87 with pH? (HPLC)
log Kow for L070296 = -2.11 with pH? (HPLC)
log Kow for L070297 = -3.62 with pH? (HPLC)
log Kow for L070298 = -1.64 with pH? (HPLC)
S > 200 mg/L to > 10 g/L at 20 °C (P)
vp < 1.0E-6 mm Hg or torr at 25 °C (P)
bp = 460 °C (P)
H for the covalent ion pair = 1.2E-7 to 9.5E-7 (P)
log Koc for the covalent ion pair = 1.4 to 2.0 (P)
log fish BCF = 0.50 (P)
sorption to sludge = low (P)

test data for L070271 for aerobic biodegradation in seawater at 20 C, via closed bottle (OECD306) were:

time (d)	biodegradation (percent)
5	0
14	2
28	63

test data for aerobic biodegradation for the [REDACTED] of L070299 from [REDACTED] were:

15% biodegradation in 28 d, thus, not readily biodegradable via CO₂ evolution in modified Sturm test (OECD301B); if test result is due solely to ester hydrolysis and degradation of the [REDACTED] moiety, then removal via POTW of the parent would be >= 90% but notifier did not measured degradation products;

POTW removal = 0% to 90 via sorption and possible biodegradation time for complete ultimate aerobic biodegradation = weeks to => months

sorption to soils and sediments = low (P)

PBT Potential: P2B1T2 to P3B1T2

*CEB FATE: migration to ground water = rapid

HEALTH: Absorption nil thru skin based on physical/chemical properties; good thru lungs based on analogs; and good thru the GI tract based on analogs;

test data for the [REDACTED] of L070299, [REDACTED], were:

rat acute oral LD₅₀ = 800 mg/kg with toxic signs; LD₁₀₀ = 2 g/kg, LD₀ = 300 mg/kg;

rat acute dermal LD₀ = 2.0 g/kg with no toxic signs; slight and transient (2 d) skin irritation in rabbits; slight and transient (1 d) eye irritation in rabbits; Ames test was negative;

E. coli test was negative;

chromosome aberration test with V79 cells was positive with activation, but negative without activation;

no skin sensitization in guinea pigs (M&K);

rat 28-d subchronic oral-gavage with doses = 1000, 300, and 100 mg/kg/d with NOAEL = 100 mg/kg/d and LOEL = 300 mg/kg/d based on salivation and increased water consumption; effects at 1000 mg/kg/d were slight to severe salivation, unsteady gait, motor activity significantly decreased and effects to the liver and kidneys;

concern for asthma and developmental toxicity based on data for benzoic acid, note: the mechanism for the asthma is unknown;

concern for possible mutagenicity, liver toxicity, and kidney toxicity based on data for [REDACTED] which was the [REDACTED] of L070299, however, the [REDACTED] will have some acylating activity

which is absent in the acid, thus, the acid will be less toxic than the [REDACTED];

low to moderate concern for toxicity

*CEB HEALTH: Exposures to humans: inhalation, ingestion, and drinking water;

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	>	100.0	P
SW fish 96-h LC50	=	440.0	M S,N L070271
SW fish 96-h LC50	>	320.0	M S,N L070290
SW fish 96-h LC50	>	320.0	M S,N L070291
daphnid 48-h LC50	>	100.0	P
SW invert Ac ton 48-h LC50	=	2830.0	M S,N L070271
SW invert Ac ton 48-h LC50	=	1500.0	M S,N L070290
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070291
SW invert Ac ton 48-h LC50	=	480.0	M S,N L070292
SW invert Ac ton 48-h LC50	=	270.0	M S,N L070293
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070294
SW invert Ac ton 48-h LC50	=	250.0	M S,N L070295
SW invert Ac ton 48-h LC50	=	300.0	M S,N L070296
SW invert Ac ton 48-h LC50	=	430.0	M S,N L070297
SW invert Ac ton 48-h LC50	=	440.0	M S,N L070298
SW invert Ac ton 48-h LC50	=	170.0	M S,N L070299
SW invert Ac ton 48-h LC50	=	130.0	M S,N L070300
green algal 96-h EC50	>	100.0	P
SW algae Sk cost 72-h EC50 c	=	250.0	M S,N L070271
SW algae Sk cost 72-h EC50 r	>	10000.0	M S,N L070290
SW algae Sk cost 72-h EC50 r	=	430.0	M S,N L070291
SW algae Sk cost 72-h EC50 r	=	660.0	M S,N L070292
SW algae Sk cost 72-h EC50 r	=	2100.0	M S,N L070296
SW algae Sk cost 72-h EC50 r	=	1500.0	M S,N L070297
SW algae Sk cost 72-h EC50 r	=	700.0	M S,N L070300
fish chronic value	>	10.0	P
daphnid ChV	>	10.0	P
algal ChV	>	10.0	P
SW algae Sk cost ChV c	=	100.0	M S,N L070271
SW algae Sk cost ChV r	=	5600.0	M S,N L070290
SW algae Sk cost ChV r	<	100.0	M S,N L070291
SW algae Sk cost ChV r	=	320.0	M S,N L070292
SW algae Sk cost ChV r	=	1000.0	M S,N L070296
SW algae Sk cost ChV r	=	320.0	M S,N L070297
SW algae Sk cost ChV r	=	320.0	M S,N L070300
benthic			
SW invert Coror vol 10-d LC50	=	6558.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d NOEC	=	470.0	mg/kg DWT M S,N L070271
SW invert Coror vol 10-d LC50	=	7300.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070290
SW invert Coror vol 10-d LC50	=	3800.0	mg/kg DWT M S,N L070291
SW invert Coror vol 10-d NOEC	=	150.0	mg/kg DWT M S,N L070291

SW invert Coror vol 10-d LC50	=	6700.0	mg/kg DWT M S,N L070292
SW invert Coror vol 10-d NOEC	=	1400.0	mg/kg DWT M S,N L070292
SW invert Coror vol 10-d LC50	=	410.0	mg/kg DWT M S,N L070296
SW invert Coror vol 10-d NOEC	=	130.0	mg/kg DWT M S,N L070296
SW invert Coror vol 10-d LC50	=	330.0	mg/kg DWT M S,N L070297
SW invert Coror vol 10-d NOEC	=	160.0	mg/kg DWT M S,N L070297
SW invert Coror vol 10-d LC50	=	280.0	mg/kg DWT M S,N L070300
SW invert Coror vol 10-d NOEC	=	16.0	mg/kg DWT M S,N L070300

Predictions are based on SARs for neutral organic chemicals with 10X less toxicity due to the substitution of the acid, or SARs for anionic surfactants-carboxylic acid-C4.Na; SAR chemical class = surfactant-anionic-F1 to F4 and CF3 benzene-COO.Na; MW162 to 216; solids with mp for L070271 (F) = 126 °C (M); log Kow for the free acid = 1.8 to 2.9 (ClogP), 1.2 to 2.8 (EPI), 1.59 to 3.10 (M); log Kow for L070271 = -5.87 with pH? (HPLC); S > 200 mg/L at 20 °C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO₃; and TOC <2.0 mg/L; low concern for toxicity

assessment factor = 10.0
concern concentration = 1.0 mg/L (ppm)
*CEB ECOTOX: No releases to water;

P2REC: forward to FOCUS with support.

SAT Co-chair: Vince Nabholz, 564.8909

GTOX Report

PMN No. L-07-0290 CAS No. 006185-28-0 Rcvd: 06/18/07 OECD Incomplet ID: Rec# 4 : 854
S/A Name of Analog S Reviewer ked

	with activation	without activation	Positive Strains
<u>Salmonella Assay:</u>	<input type="checkbox"/>	<input type="checkbox"/>	
<u>Chromosomal Aberration</u>	<u>CHO:</u> <input type="checkbox"/>	<input type="checkbox"/>	
	<u>CHL:</u> <input type="checkbox"/>	<input type="checkbox"/>	
	<u>V79:</u> <input type="checkbox"/>	<input type="checkbox"/>	
<u>E. coli Reverse Mutation:</u>	<input type="checkbox"/>	<input type="checkbox"/>	
<u>Mouse Micronucleus Assay:</u>	Route: <input type="text"/>	<input type="checkbox"/>	
<u>Rat Hepatocytes Unscheduled DNA Synthesis:</u>		<input type="checkbox"/>	

Other GTOX Results

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Comments

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ECOTOX: X

Fate:

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WS/Log P:

LogP=-5.2, p.27

NCSAB SAT REPORT

PMN: L-07-0290

CAS RN:

6185-28-

Chemical Name:

Benzoic acid, 2,6-difluoro-, sodium salt (1:1)

Analogs:

Production Volume:

1000.00

Structure:



Use: chemical to measure flow in deep oil-bearing strata.

Concurrently submitted similar cases L-07-290 and L-07-292 to L-07-295.

Analog L-07-271 has this same use. There is one reference in file CA on STN, a toxicity study.

P2REC: CRSS: forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata. The LVE substance has been awarded Offshore Chemical Notification System Gold

Formula: C₇H₃F₂NaO₂ Eq Wt:

Mol Weight: 180.09 Wt%<500: Wt%<1000

MP: BP: >500 VP: <0.000001

H₂O Sol (g/L): >200 Physical State: Solid Log P:

Endpoint (mg/L) Est. Value Meas. Value Comments

Fish 96-h >100

Daphnid 48-h >100

Algal 96-h >100

Fish ChV >10

Daphnid ChV >10

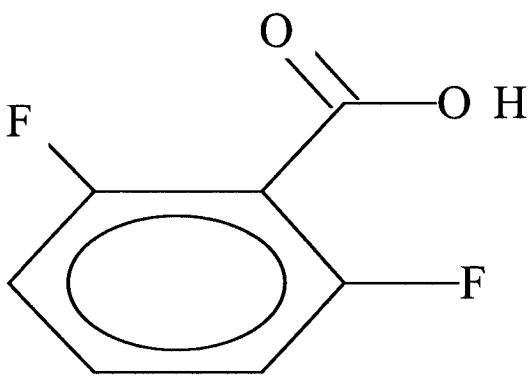
Algal ChV >10

BCF

CHEMICAL CLASS: SAR:

ECOTOX CONCERN H M C CONCERN CONCENTRATION >1.0

DATE 6/29/07 ASSESSOR:



SMILES : Fc1ccccc(F)c1C(=O)(O)
 CHEM :
 CAS Num:
 ChemID1:
 ChemID2:
 ChemID3:
 MOL FOR: C7 H4 F2 O2
 MOL WT : 158.11
 Log Kow: 1.76 (User entered)
 Melt Pt: 160.00 deg C
 Wat Sol: 227 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

 Neutral Organics-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	343.547 *

--> Acid moiety found: Predicted values multiplied by 10

Neutral Organics-acid	: Fish	96-hr	LC50	1970.364 *
Neutral Organics-acid	: Fish	14-day	LC50	3435.472 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	2076.569 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	1280.402 *
Neutral Organics-acid	: Fish	30-day	ChV	244.200 *
Neutral Organics-acid	: Daphnid	16-day	EC50	95.884
Neutral Organics-acid	: Green Algae	96-hr	ChV	111.457
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	401.926 *
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	674.445 *

Neutral Organics-acid	: Earthworm	14-day	LC50	mg/kg (ppm) dry wt soil =====
				11530.985 *

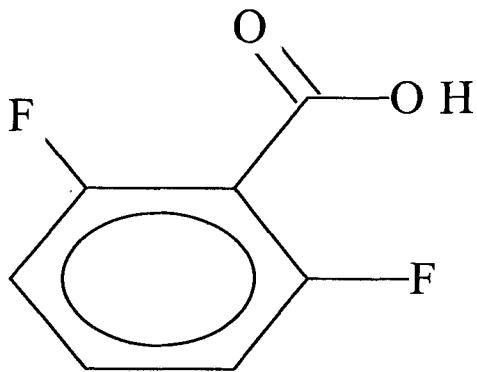
Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000



SMILES : Fc1ccccc(F)c1C(=O)(O)

CHEM :

MOL FOR: C7 H4 F2 O2

MOL WT : 158.11

----- EPI SUMMARY (v3.12) -----

Physical Property Inputs:

Water Solubility (mg/L) :	-----	Log Kow (oct-water):	1.76
Vapor Pressure (mm Hg) :	-----	Boiling Pt (deg C):	-----
Henry LC (atm-m ³ /mole) :	-----	Melting Pt (deg C):	160.00

Log Kow (KOWWIN v1.67 estimate) = 1.18 Exp database: 1.59

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):

Boiling Pt (deg C):	241.34		
Melting Pt (deg C):	47.62	MP(exp database):	159 deg C
VP(mm Hg, 25 deg C):	0.00171		

Water Solubility estimate (WSKOW v1.41): 2301 mg/L

Water Solubility estimate (fragments): 6599.1 mg/L

Henry's Law Constant (atm-m³/mole) [HENRYWIN v3.10]:

Bond Method:	1.48E-007	Group Method:	3.62E-007
Henry's LC [VP/WSol estimate using EPI values]:	1.546E-007 atm-m ³ /mole		

Biodegradation Estimates (BIOWIN v4.02):

Atmospheric Oxidation (25 deg C) [AopWin v1.91]:

OH Half-Life =	6.471 Days (12-hr day; 1.5E6 OH/cm ³)
No Ozone Reaction Estimation	

Soil Adsorption (PCKOCWIN v1.66): Koc = 39.61 Log Koc = 1.598

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF estimate (BCFWIN v2.15): Log BCF = 0.500 (BCF = 3.162)

Volatilization from Water: (Henry LC = 3.62e-007 atm-m³/mole)
Half-Lives: Model River = 2035 hr, Model Lake = 2.231e+004 hr

Removal In Wastewater Treatment (percents, 99% recommended maximum):

TOTAL: 2.10, Biodeg: 0.09, Sludge: 1.98, Air: 0.02

Level III Fugacity Model (conc %, half-life hr):

Air(1.44%,155), Water(33%,1.44e+003), Soil(65.4%,2.88e+003), Sediment(0.102%,1.3e+004)
Persistence Time: 1.17e+003 hr

CHEMICAL: Unknown
MOL WT : 158.11
MOL FOR: C7H4F2O2
SMILES : Fc1cccc(F)c1C(=O)=O
ISOC-ID: -a-aaaa---a-----
FRAG-ID: 1_____2____3_3_3
H-COUNT: ____111_____1

10:04:58 06/27/:7

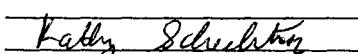
Class	Type	Contribution Description	Comment	Value
FRAGMENT	# 1	Fluoride	MEASURED	0.370
FRAGMENT	# 2	Fluoride	MEASURED	0.370
FRAGMENT	# 3	Carboxy (ZW-)	MEASURED	-0.030
ISOLATING	CARBON	6 Aromatic isolating carbon(s)		0.780
EXFRAGMENT	HYDROG	3 Hydrogen(s) on isolating carbons		0.681
ELECTRONIC	SIGRHO	2 Potential interactions; 1.50 used	withinRing	0.147
ORTHO	RING 1	2 Normal ortho interaction(s)		-0.560
RESULT	v3.3	All fragments measured	ESTIMATE	1.758

ATTENDEES

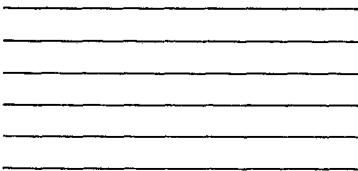
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CHEMISTRY

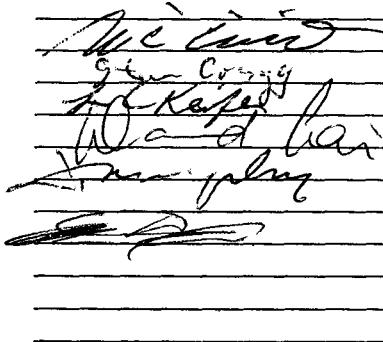
- Paul Bickart
 Diana Darling
 Rich Engler
 Greg Fritz
 Daniel Lin
 Kathy Schechter

**ENVIRONMENTAL FATE**

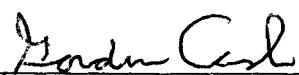
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 Wen-Hsiung Lee
 Laurence Libelo
 David Lynch
 Andy Mamantov

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 Michael Cimino
 Steve Cragg
 Leonard Keifer
 David Lai
 Jim Murphy
 Deborah Norris
 Ronald Ward
 Yin Tak Woo

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 Vince Nabholz
 Maggie Wilson

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- Rebecca Jones
 Leonard Keifer
 Vince Nabholz
 Jim Kwiat

